Cristine Villagonzalo · Rayda Gammag

The intrinsic features of the specific heat at half-filled Landau levels of two-dimensional electron systems

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Abstract The specific heat capacity of a two-dimensional electron gas is derived for two types of the density of states, namely, the Dirac delta function spectrum and that based on a Gaussian function. For the first time, a closed form expression of the specific heat for each case is obtained at half-filling. When the chemical potential is temperature-independent, the temperature is calculated at which the specific heat is a maximum. Here the effects of the broadening of the Landau levels are distinguished from those of the different filling factors. In general, the results derived herein hold for any thermodynamic system having similar resonant states.

Keywords Two-dimensional electron gas \cdot Density of states \cdot Landau levels \cdot Specific heat

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1 Introduction

Electrons in a two-dimensional layer continue to be of interest in physics since they exhibit nonclassical behavior and are readily realizable in semiconductor

C. Villagonzalo · R. Gammag Structure and Dynamics Group National Institute of Physics, University of the Philippines, Diliman, 1101 Quezon City, Philippines

Tel.: +632-920-9749 Fax: +632-928-0296

C. Villagonzalo

E-mail: cvillagonzalo@nip.upd.edu.ph

R. Gammag

E-mail: rayda.gammag@up.edu.ph

heterostructures [1]. Nowadays research investigations on two-dimensional electron gas (2DEG) systems are aimed at understanding the plateaus in the quantum Hall conductance [2] and the de Haas - van Alphen effect or the magnetization oscillations [3,4,5]. The smooth drop of the plateaus and the extrema of the oscillations reveal broadened energy levels, that is, a finite density of states (DOS) [6] between eigenvalues E_n . These E_n , known as Landau levels, are the quantized energy spectrum (E) obtained when a strong magnetic field (B) is applied perpendicular to the system's plane [7] or in a tilted direction relative to it [8]. The striking behavior of E_n broadening, from which other exotic features arise, has been attributed to disorder due to the presence of impurities, defects and other inhomogeneities in the system [9,10,11].

Ideally, the DOS of a noninteracting 2DEG in a perpendicular B is given as a series of delta functions [7], that is,

$$D(E) = \frac{2eB}{h} \sum_{n} \delta(E - E_n) . \tag{1}$$

Here e is the electron charge, h is Planck's constant and $E_n = (n+1/2)\hbar\omega_c$ is the nth Landau energy level. The latter depends on B through the cyclotron frequency $\omega_c = eB/m^*$ for a given effective mass m^* . Such a DOS structure can be used to model actual materials with a very narrow distribution of energy carriers [3].

Usually, the actual shape of the density of states of a 2DEG is determined by making theoretical fits to the heat capacity data from experimental measurements. This procedure made on a 2DEG in GaAs-GaAlAs multilayers [12], for instance, yields a DOS with Gaussian peaks on a flat background. Many experimental and theoretical studies on the thermodynamic and magnetic properties of 2DEG systems, therefore, use a form of DOS based on a Gaussian function [7,11,13,14] such as

$$D(E) = \frac{2eB}{h} \sum_{n} \left(\frac{1}{2\pi}\right)^{1/2} \frac{1}{\Gamma} \exp\left[-\frac{(E - E_n)^2}{2\Gamma^2}\right] , \qquad (2)$$

where the broadening is taken into account by the parameter Γ .

In one study using this DOS, the authors of Ref. [14] predicted that the specific heat and other magneto-thermal effects at high B become universal functions of k_BT/Γ , where k_B is the Boltzmann's constant and T is the temperature. However, their numerical calculations at constant electron concentration were unable to provide the exact dependence of these thermodynamic properties on k_BT/Γ .

Another study of an impurity-free quantum Hall system in a periodic rectangular geometry found that the specific heat at constant volume behaves as $C_V \propto \exp[-\Delta/T]/T^2$, where Δ is the energy gap between the ground state and the first excited state [16]. The numerical calculations in Ref. [16] derived C_V for different values of the filling factor ν . This nominal number of filled Landau levels is given as $\nu = hN/Be$, where N is the electron concentration. For various filling factors, their results yield a C_V with a sharp peak at low T whose height depends on Δ . However, their C_V calculations show that

finite size effects become dominant at low T. Without an exact expression for C_V , it would also be difficult to distinguish the $\exp[-\Delta/T]/T^2$ behavior from the dominant lattice contribution $\sim T^3$ at very low T. In general, since C_V depends strongly on the nature of a given system such as the DOS, the exact behavior of C_V as a consequence of its electronic structure is not easily determined.

In this work, the authors will show that a closed form expression of C_V is obtained for a 2DEG system when the chemical potential μ does not vary with T. The latter condition is satisfied at a finite non-zero T when the last occupied Landau level is half-filled, that is, the last occupied energy level is filled to half its degeneracy. Particular interest has been devoted to $\nu = 1/2$ and other half-filled states since no plateau of the Hall resistance is observed unlike other fractional ν with an odd denominator [17]. At half-filling, the chemical potential is right at the center of the Landau level where extended states are located [2]. There is an absence of a gap at this ν and some experiments have observed features of a Fermi-liquid state [18,19].

Here a detailed derivation will be presented of C_V at $\nu=n'/2$ (where n' is an odd integer) for a spinless 2DEG having a delta-shaped or a Gaussian DOS in the presence of a perpendicular applied magnetic field. The exact relations for the specific heat as obtained for the first time in this work serve as a basis that characterizes the underlying density of states of an electron gas. In addition, the condition at which the heat capacity is a maximum is established for both cases including the actual nature of its dependence on Γ . This will be particularly useful for the design of devices that are intended to resist changes in temperature. Lastly, remarks will also be given regarding C_V at other filling factors and hence, the general case will be formulated.

2 The Temperature Dependence of the Chemical Potential

The chemical potential μ , which measures the amount of energy required to add a particle in a given system, is generally a function of T and B. But at half-filling the μ is independent of T since the 2DEG is metallic and there is no energy gap between the conduction and the valence bands. This is demonstrated in Fig. 1. The chemical potential shown here is obtained for a fixed electron concentration.

$$N = \int f(E)D(E) dE, \qquad (3)$$

using the root-finding method as outlined in Ref. [15]. Here f(E) is the Fermi-Dirac distribution function and it is given as

$$f(E) = \frac{1}{\exp[(E - \mu)/k_B T] + 1} . \tag{4}$$

The value of N is set equal to 3.6×10^{11} cm⁻², which has the same order of magnitude as in experiments of 2DEG systems in semiconductors. In addition, the 2DEG system used has a Gaussian DOS as given in Eq. (2) with $\Gamma = 0.2$ meV. No spin-splitting is considered here. Hence, in Fig. 1

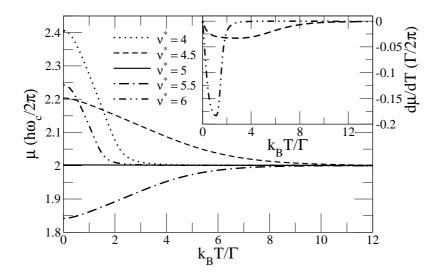


Fig. 1 The temperature-dependent chemical potential at various filling factors for a 2DEG system with a Gaussian DOS. Here $\nu^* = 5$ corresponds to half-filling for spinless electrons. This illustrates that μ does not change with T in this case. As examples, the inset provides the derivative of μ with respect to T for $\nu^* = 4.5$ and $\nu^* = 6$.

the even integer ν^* corresponds to full filling and the odd integer ν^* to half-filling, that is, $\nu^*/2 \to \nu$. As the T approaches zero, the μ of the fully-filled states ($\nu^*=4$, 6) varies within $\hbar\omega_c/2$ from the temperature-independent μ ($\nu^*=5$). This is likewise observed for the non-half partially filled states ($\nu^*=4.5, 5.5$), albeit at a gradual slope. This signifies that the μ behavior and, consequently, the specific heat nature of 2DEG systems at the non-half-filled states can be considered as deviations from their behavior at half-filling. In fact, the μ saturates to its half-filling value as T increases. Treating the μ as T-independent is a valid approximation even for non-half-fillings albeit limited only at high T.

3 The Heat Capacity at Half-Filling

The specific heat of a substance is a measure of the amount of energy needed to raise its temperature by a degree. For an electron gas at constant volume, C_V can be obtained from its internal energy U as follows

$$C_V = \frac{\partial U}{\partial T} = \frac{\partial}{\partial T} \int_{-\infty}^{\infty} f(E)(E - \mu)D(E)dE . \tag{5}$$

When the μ does not vary with T, only the f(E) remains as the T-dependent function. The temperature derivative in Eq. (5) then acts only on

f(E) and Eq. (5) can be rewritten as

$$C_V = k_B \int_{-\infty}^{\infty} \frac{[(E - \mu)/2k_B T]^2}{\cosh^2[(E - \mu)/2k_B T]} D(E) dE.$$
 (6)

3.1 For a Delta-shaped DOS

As shown in the numerical calculations of Ref. [15] at constant N, despite the presence of the broadening of Landau levels, a characteristic low temperature is reached at which the 2DEG approaches its ideal electron gas behavior. Therefore, the continued use of a delta-shaped DOS is justified in heat capacity measurements at strong B and below a characteristic low T.

Substituting D(E) of Eq. (1) in Eq. (6), we obtain the specific heat at half-filling for a delta-shaped DOS, that is,

$$C_V = k_B \frac{2eB}{h} \sum_n \frac{[(E_n - \mu)/2k_B T]^2}{\cosh^2[(E_n - \mu)/2k_B T]} . \tag{7}$$

Note that the number of occupied Landau levels and the chemical potential are determined if the electron concentration is known. For this case, the contribution of the last occupied Landau level, $n = n_{max}$, to the C_V is zero since $E_n = \mu$.

The specific heat expressed in Eq. (7) exhibits a single peak at the low temperature region. The temperature at which C_V is a maximum can be obtained by taking $\partial C_V/\partial T=0$ and performing a second-derivative test. The non-trivial condition at which this is satisfied is when

$$\sum_{n} \omega_n \frac{\tanh(\omega_n)}{\cosh^2(\omega_n)} \left[(\omega_n) - \coth(\omega_n) \right] = 0 , \qquad (8)$$

where $\omega_n = (E_n - \mu)/2k_BT$ and $E_n \neq \mu$. The maximum specific heat becomes

$$C_{V, max} = k_B \frac{2eB}{h} \sum_{n=0}^{n_{max}-1} \frac{1}{\sinh^2[(E_n - \mu)/2k_B T]}$$
 (9)

The value of T when C_V is a maximum, $T_{\rm peak}$, can be determined at $n=n_{max}-1$ because this is the most dominant term. Also, $E_{n_{max}-1}\neq\mu$ and Eq. (8) remains valid. At this level, solving for $\omega_n-\coth(\omega_n)=0$ yields $\omega_n=1.19968$. Thus, we find that $T_{\rm peak}\simeq 0.416778(E_{n_{max}-1}-\mu)/k_B$. This result also provides a measure of the Landau level spacing.

The derivations herein are valid for any B and for any $\mu(B)$ as long as the condition of half-filling is met or whenever the chemical potential does not change with temperature.

3.2 For a Gaussian-shaped DOS

There are other forms of the density of states used in the literature [3,4, 12] such as the Lorentzian, Gaussian with a constant background and the semielliptical distribution function. Here we consider only the Gaussian DOS as given in Eq. (2) to demonstrate the effect of a finite broadening Γ as compared to the ideal impurity-free case. We keep in mind that in the limit as the $\Gamma \to 0$, the Gaussian DOS approaches the delta-shaped DOS as given in Eq. (1) since

 $\delta(x) = \lim_{\Gamma \to 0} (1/2\pi\Gamma^2)^{1/2} \exp(-x^2/2\Gamma^2).$ Substituting Eq. (2) in Eq. (6) yields

$$C_V = \frac{k_B}{\Gamma} \frac{2eB}{h} \left(\frac{1}{2\pi}\right)^{1/2} \sum_n \int_{-\infty}^{\infty} \exp\left(-\frac{(E - E_n)^2}{2\Gamma^2}\right) \times \frac{[(E - \mu)/2k_BT]^2}{\cosh^2[(E - \mu)/2k_BT]} dE.$$
 (10)

For clarity and brevity, dimensionless energy parameters $\omega = (E-\mu)/2k_BT$ and $\omega_n = (E_n - \mu)/2k_BT$ are introduced such that the specific heat given in Eq. (10) reduces to

$$C_V = \frac{k_B}{\gamma} \frac{2eB}{h} \left(\frac{1}{\pi}\right)^{1/2} \sum_n \int_{-\infty}^{\infty} \exp\left[-\frac{(\omega - \omega_n)^2}{\gamma^2}\right] \times \left[\frac{\omega}{\cosh(\omega)}\right]^2 d\omega . (11)$$

Here $\gamma = (1/2)^{1/2} \Gamma / k_B T$ is the dimensionless broadening parameter.

The integral in the specific heat expression, Eq. (11), is evaluated in two sequences of integration by parts which involve the integrals from Ref. [20]: that is, (i) following Integral No. 8 of Section 2.477 [20]

$$\int \frac{\omega^2}{[\cosh(\omega)]^2} d\omega = \omega^2 \tanh(\omega) - 2\sum_{k=1}^{\infty} \frac{2^{2k}(2^{2k} - 1)B_{2k}}{(2k+1)(2k)!} \omega^{2k+1} , \quad (12)$$

and that of (ii) Integral No. 7 of Section 2.479 [20]

$$\int \omega^p \tanh(\omega) \, d\omega = \sum_{k=1}^{\infty} \frac{2^{2k} (2^{2k} - 1) B_{2k}}{(p+2k)(2k)!} \omega^{p+2k} \,, \tag{13}$$

where $|\omega| < \pi/2$ and p > -1. The constant B_{2k} is the 2k-th Bernoulli number. The infinite integration of products of powers and hyperbolic functions are best treated using the Bernoulli series as a generating function in regions where the hyperbolic functions converge.

In terms of these integrals, the specific heat for a Gaussian DOS is given as

$$C_{V} = \frac{k_{B}}{\gamma} \frac{2eB}{h} \left(\frac{1}{\pi}\right)^{1/2} \sum_{n} \left\{ \left[\exp\left[-\frac{(\omega - \omega_{n})^{2}}{\gamma^{2}} \right] \times \left(\omega^{2} \tanh(\omega) + \sum_{k=1}^{\infty} \frac{2^{2k+1}(2^{2k} - 1)B_{2k}}{(2k)!} \right) \right] \times \left[-\frac{\omega^{2k+1}}{2k+1} + \frac{1}{\gamma^{2}} \frac{\omega^{2k+3}}{2k+3} - \frac{\omega_{n}}{\gamma^{2}} \frac{\omega^{2k+2}}{2k+2} \right] \right]_{\omega = -\pi/2}^{\omega = \pi/2} + \frac{1}{\gamma^{2}} \sum_{k=1}^{\infty} \frac{2^{2k+2}(2^{2k} - 1)B_{2k}}{(2k)!} \left[\int_{-\pi/2}^{\pi/2} \exp\left[-\frac{(\omega - \omega_{n})^{2}}{\gamma^{2}} \right] (\omega - \omega_{n}) \left(-\frac{\omega^{2k+1}}{2k+1} - \omega_{n} \frac{\omega^{2k+2}}{2k+2} + \frac{\omega^{2k+3}}{2k+3} \right) d\omega \right] \right\}.$$
 (14)

The remaining integrals in Eq. (14) are of the form

$$\int_{-\pi/2}^{\pi/2} \exp\left[-\frac{(\omega - \omega_n)^2}{\gamma^2}\right] \,\omega^s \,d\omega = \sum_{j=0}^s \frac{s!}{j!(s-j)!} \omega_n^{s-j} \gamma^{j+1} \,F(j) \,\,, \quad (15)$$

where for the case when j is odd

$$F(j) = -\frac{[(j-1)/2]!}{2} \exp\left(-\frac{(\omega - \omega_n)^2}{\gamma^2}\right) \sum_{l=0}^{(j-1)/2} \frac{1}{l!} \left(\frac{\omega - \omega_n}{\gamma}\right)^{2l} \bigg|_{\omega = -\pi/2}^{\omega = \pi/2}$$
(16)

and for the case when j is even

$$F(j) = \left\{ -\exp\left[-\frac{(\omega - \omega_n)^2}{\gamma^2} \right] \sum_{l=0}^{j/2-1} \frac{(j-1)!!}{2^{j/2-l}(2l+1)!!} \times \left(\frac{\omega - \omega_n}{\gamma} \right)^{2l+1} + \frac{(j-1)!!}{2^{j/2+1}} (\pi)^{1/2} \operatorname{erf} \left[\frac{\omega - \omega_n}{\gamma} \right] \right\}_{\omega = -\pi/2}^{\omega = \pi/2} .$$
 (17)

In this equation, $\operatorname{erf}[z] = (2/\sqrt{\Pi}) \int_0^z \exp[-z^2] \, dz$ is the error function. The series and integrals of Eq. (14) converge. Therefore, one can determine the exact value of C_V at a given T and B for a particular γ .

Note that, at half-filling, $E_n = \mu$ at the last occupied Landau level, $n = n_{max}$. In these cases, $\omega_n = 0$. Hence, the integral of Eq. (15) vanishes. Therefore, the specific heat at the last occupied Landau level given by Eq. (14) evaluated from $\omega = -\pi/2$ to $\omega = \pi/2$ at $\omega_n = 0$ yields

$$C_{V, n_{max}} = \frac{2eB}{h} \left(\frac{1}{\pi}\right)^{1/2} \frac{k_B}{\gamma} \left\{ \exp\left[-\left(\frac{\pi}{2\gamma}\right)^2\right] \times \left(\frac{1}{2}\pi^2 \tanh\left(\frac{\pi}{2}\right) + \frac{1}{\gamma^2}C_1 - C_2\right) \right\},$$
(18)

where the coefficients C_1 and C_2 are constants. From Eq. (14), these constant coefficients are derived to be as follows

$$C_1 = \frac{1}{2} \sum_{k=1}^{\infty} \frac{(2^{2k} - 1)B_{2k}}{(2k+3)(2k)!} \pi^{2k+3} , \qquad (19)$$

and

$$C_2 = 2\sum_{k=1}^{\infty} \frac{(2^{2k} - 1)B_{2k}}{(2k+1)(2k)!} \pi^{2k+1} . (20)$$

Their numerical values are $C_1 = 5.07023$ and $C_2 = 3.6412$.

Recall that γ is inversely proportional to T. Setting to zero the derivative with respect to T of Eq. (18), a quartic equation is obtained. This yields one real root with T > 0. This is the temperature at which the specific heat has a maximum at $E_n = \mu$, namely,

$$T_{peak} = \frac{\Gamma}{k_B} \left\{ -\frac{1}{8\pi^2 C_1} \left(-12C_1 - 2\pi^2 C_2 + C_3 - \left[144C_1^2 + 16\pi^2 C_1 C_2 + 4\pi^4 C_2^2 - 8C_1 C_3 - 4\pi^2 C_2 C_3 + C_3^2 \right]^{1/2} \right) \right\}^{1/2}, (21)$$

where $C_3 = \pi^4 \tanh[\pi/2] = 89.339$. This yields that $T_{\rm peak} = 0.501815 \ \Gamma/k_B$. It is important to focus on the last occupied Landau level at $n = n_{max}$ at high B and low T because this is where the significant contribution to C_V comes from [13]. Since we are considering half-filling, $E_{n_{max}} = \mu$, the specific heat as derived from Eq. (10) becomes Eq. (18). When this is rewritten in terms of $k_B T/\Gamma$, we find that

$$C_{V, n_{max}} = k_B \frac{2eB}{h} \left(\frac{1}{\pi}\right)^{1/2} \exp\left[-\frac{\pi^2}{2} \left(\frac{k_B T}{\Gamma}\right)^2\right] \times \left(2^{1/2} \left[\frac{1}{2} \pi^2 \tanh\left(\frac{\pi}{2}\right) - C_2\right] \frac{k_B T}{\Gamma} + 2^{3/2} C_1 \left[\frac{k_B T}{\Gamma}\right]^3\right), \tag{22}$$

where the coefficients C_1 and C_2 are constants. They are given in Eq. (19) and Eq. (20), respectively. This result is consistent with the case for bulk metals that the $C_V \sim aT + bT^3$ where a and b are arbitrary coefficients. The linear in T behavior of C_V comes from the electronic contribution, while the T^3 behavior is associated with lattice vibrations. This broadening of the Landau levels as represented by a Gaussian DOS that yields the T^3 contribution to the specific heat may be in part of the same nature as phonons. In addition to the similarity with metallic bulk properties, we obtain a Gaussian dependence on k_BT/Γ for the specific heat as a natural consequence of the DOS, that is, $C_V \sim \exp[-(k_BT/\Gamma)^2]$. This is unlike in Ref. [16] where $C_V \sim \exp[-\Delta/T]$. Thus, in this work, the drop in C_V after the $T_{\rm peak}$ is caused by the Gaussian tail

Equation (22) serves as a reference for the C_V measurement as Γ is varied. When Γ is comparable to or greater than k_BT , C_V decreases as Γ increases for a given T. This is due to the lesser energy requirement to move from one

energy level to the next since there is a larger overlap between neighboring Landau levels. When $\Gamma << k_B T$, the exponential behavior of Eq. (22) dominates. In this case, C_V increases as Γ increases. We have assumed here that Γ is a constant for a given B and T. Also, Γ is assumed to be the same for all Landau levels. However, the effect of Γ will be balanced by an increasing B that increases the separation between Landau levels while raising the degeneracy of the states. Even when a B-dependent critical value of Γ is reached wherein the blend of states disappear [8], the expression for $C_{V, n_{max}}$ will still hold.

Furthermore, the functional form of C_V in Eq. (22) yields a single peak. As obtained from Eq. (21), this occurs at $T_{\rm peak} = 0.501815~\Gamma/k_B$. This linear proportionality with $T_{\rm peak}$ and Eq. (22) can be used to directly measure the broadening parameter of the DOS for a given B whenever experimental data for the C_V in a 2DEG system are available.

4 A Note on the General Case

When the chemical potential is temperature-dependent, the derivative of the Fermi function is of the general form

$$\frac{\partial f}{\partial T} = -\frac{\partial f}{\partial E} \left[\frac{E - \mu}{T} + \frac{\partial \mu}{\partial T} \right] . \tag{23}$$

This will yield two terms in the specific heat as given in Refs. [13,14]. But aside from f(E), the specific heat also has an explicit dependence on $\partial \mu/\partial T$. Evaluating the temperature derivative in Eq. (5) results into

$$C_V = \int_{-\infty}^{\infty} \frac{\partial f(E)}{\partial T} (E - \mu) D(E) dE - \int_{-\infty}^{\infty} f(E) \frac{\partial \mu}{\partial T} D(E) dE .$$
 (24)

Using in this expression the Eq. (23), we obtain the detailed formula for C_V when $\mu = \mu(T)$ as follows

$$C_V = k_B \int_{-\infty}^{\infty} \frac{[(E-\mu)/2k_B T]^2}{\cosh^2[(E-\mu)/2k_B T]} D(E) dE$$

$$+ \frac{\partial \mu}{\partial T} \left[\frac{1}{2} \int_{-\infty}^{\infty} \frac{[(E-\mu)/2k_B T]}{\cosh^2[(E-\mu)/2k_B T]} D(E) dE - \int_{-\infty}^{\infty} f(E)D(E) dE \right]$$
(25)

This is the general equation for the specific heat and is valid regardless of the filling factor used. Hence, we find that the correction to Eq. (6) for C_V will depend on how large $\partial \mu/\partial T$ is. In the case of a Gaussian-shaped DOS, we have numerically shown that the contribution from $\partial \mu/\partial T$ for a fixed concentration is small. In the example given in the inset of Fig. 1, this contribution is of the order of $0.01-0.1~{\rm meV/K}$.

In the case of the delta-shaped density of states, substituting the DOS of Eq. (1), in Eq. (25) yields

$$C_V = k_B \frac{2eB}{h} \sum_n \left\{ \frac{\omega_n^2}{\cosh^2[\omega_n]} + \frac{1}{2k_B} \frac{\partial \mu}{\partial T} \left[\frac{\omega_n}{\cosh^2[\omega_n]} - \frac{2}{\exp[2\omega_n] + 1} \right] \right\} (26)$$

where $\omega_n = (E_n - \mu)/2k_BT$. We get two corrections terms to Eq. (7). Their values depend again on the magnitude of $\partial \mu / \partial T$.

Though the focus of this work is on the 2DEG, the theoretical model as presented is also applicable for any system under the grand canonical ensemble formulation with either a delta-shape or a Gaussian-broadened density of states.

5 Conclusions

The cardinal behavior of the specific heat of two-dimensional electron gas systems in an applied perpendicular magnetic field is derived for the cases wherein the density of states either has a delta-shape or a Gaussian form. This work establishes for both cases of the DOS the leading contributions to the specific heat and the temperature condition at which the C_V is a maximum. The exact expressions obtained for C_V hold when the chemical potential is independent of the temperature or the 2DEG is in a half-filling state. At low T and when the μ depends on T, the formulation derived herein remains valid with an additional term in C_V that is proportional to the $\partial \mu/\partial T$. Furthermore, the results provide the linear proportionality of the broadening of the Landau levels to the temperature at which the C_V attains its highest value. Experimental realizations of the results for the broadening parameter can be made, for example, if it is induced by the presence of impurities, by varying impurity levels of a half-filled 2DEG system and monitoring the corresponding changes of the temperature at which the C_V is a maximum. When effects of various spin configurations are then considered, the derivations in this work can be used to distinguish them from the effects of the temperature dependence of the μ and the broadening of the Landau levels.

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